# Advances in De Novo Drug Design: From Conventional to Machine Learning Methods

Year: 2021 | Citations: 226 | Authors: Varnavas D. Mouchlis, A. Afantitis, A. Serra, Michele Fratello, A. Papadiamantis

---

## Abstract

De novo drug design is a computational approach that generates novel molecular structures from atomic building blocks with no a priori relationships. Conventional methods include structure-based and ligand-based design, which depend on the properties of the active site of a biological target or its known active binders, respectively. Artificial intelligence, including ma-chine learning, is an emerging field that has positively impacted the drug discovery process. Deep reinforcement learning is a subdivision of machine learning that combines artificial neural networks with reinforcement-learning architectures. This method has successfully been em-ployed to develop novel de novo drug design approaches using a variety of artificial networks including recurrent neural networks, convolutional neural networks, generative adversarial networks, and autoencoders. This review article summarizes advances in de novo drug design, from conventional growth algorithms to advanced machine-learning methodologies and high-lights hot topics for further development.